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FIG. 2

level 0 1 2 3 4 5 6

Diagram illustrating a hierarchical structure (likely a tree or graph) across levels 0 to 6. The structure shows nodes branching out, with labels C1, C2, Q1, Q, and H indicating different types of nodes or states. The diagram is divided into vertical sections by dashed lines corresponding to the levels.

Key components and connections:

- Level 0:** Root node C1.
- Level 1:** C1 branches into C2 and C1.
- Level 2:** C2 branches into Q1 and H. C1 branches into Q and H.
- Level 3:** Q branches into C1 and C1.
- Level 4:** The rightmost C1 branches into Q1 and H.
- Level 5:** Q1 branches into &1 and Q1.
- Level 6:** The rightmost Q1 branches into H.

Labels 11 through 14 are used to group specific nodes or branches:

- 11: Grouping the rightmost Q1 and its child H.
- 12: Grouping the C1 node at level 3 and its child Q1.
- 13: Grouping the C1 node at level 3 and its child Q1.
- 14: Grouping the C1 node at level 1 and its child Q.

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FIG. 4

CANOST (modified) code list

no	code	substructure	no.	code	substructure	no.	code	substructure
1 ^{a)}	&nc	code for ring closing	12 ^{b)}	Y		22	LF	—F
2	T	$\text{—C}\equiv$	13 ^{c)}	Y1	$\text{H—C}\langle$	23	LC	—Cl
3	T1	$\text{H—C}\equiv$	14 ^{d)}	YTT		24	LB	—Br
4	DD	=C=				25	LJ	—I
5	DS		15	V	>C=O	26	X	other atom
6	D1	H—C=	16	V1	H—C=O	27 ^{e)}	XR	$\text{X}\langle$
7	D2	$\text{H}_2\text{C=}$	17	VD	=C=O	28	XW	$\text{X}\begin{smallmatrix} \text{O} \\ \text{=O} \end{smallmatrix}$
8	C		18	QD	=O	29	XD	=X
9	C1		19	Q	=O—	30	XN	=X=
10	C2		20	Q1	—O—H	31	XT	$\equiv\text{X}$
11	C3		21	Q0	—O^-	32 ^{f)}	Xnp	XH_{np}
						33	H	—H

- a) A cn is a serial no. of the closing site.
 b) Aromatic carbon without hydrogen.
 c) Aromatic carbon with hydrogen.
 d) —C(OH)—C(O)— in troponoid.
 e) Non-carbon atom in aromatic structure.
 f) A np is the number of connecting hydrogens.

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Figure 1 illustrates the CANOST algorithm for the chemical structure of D-glucose. The process is shown in five stages:

- (a) **Starting Point**: The chemical structure of D-glucose is shown, with a starting point (C1) identified.
- (b) **Make Tree Structure**: The structure is converted into a tree structure, showing the hierarchy of atoms (C, O, H).
- (c) **Convert Each of Nodes into CANOST codes**: Each node in the tree is assigned a CANOST code (e.g., C1, Q1, C2, V1, QD).
- (d) **Rearrange in the Order of Precedence of CANOST Codes**: The codes are rearranged into a linear sequence based on their precedence.
- (e) **Convert into Linear Notation**: The linear sequence of codes is converted into a final linear notation string: `C2 * C1 ; Q1 ; H ; H * C1 ; Q ; H , , * C1 ; Q1 ; H , , * V1 ; Q1 ; H , , * QD ; H , , *`

(b)

(e)

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FIG. 6

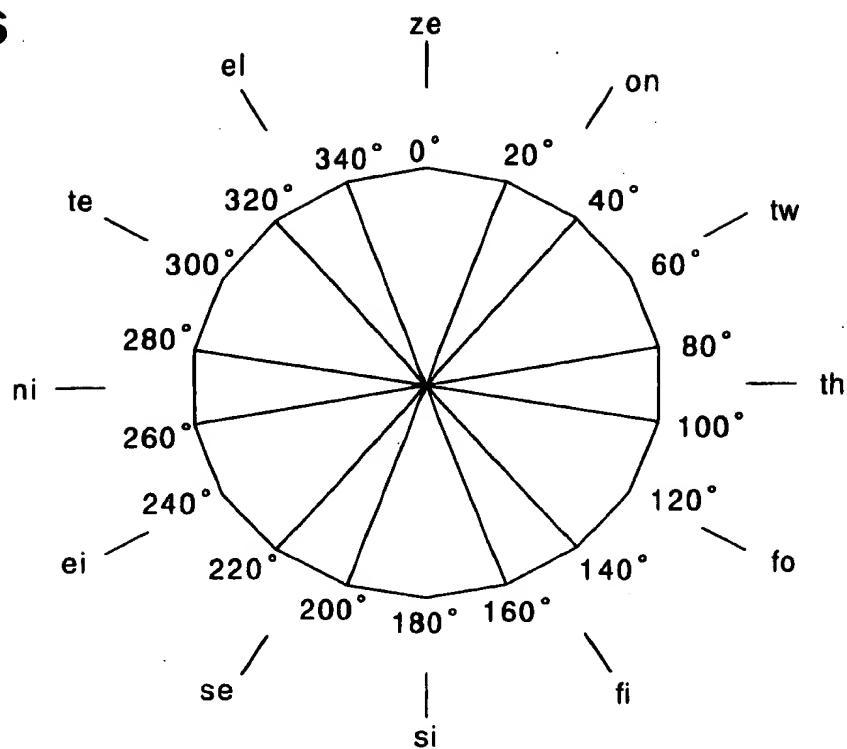
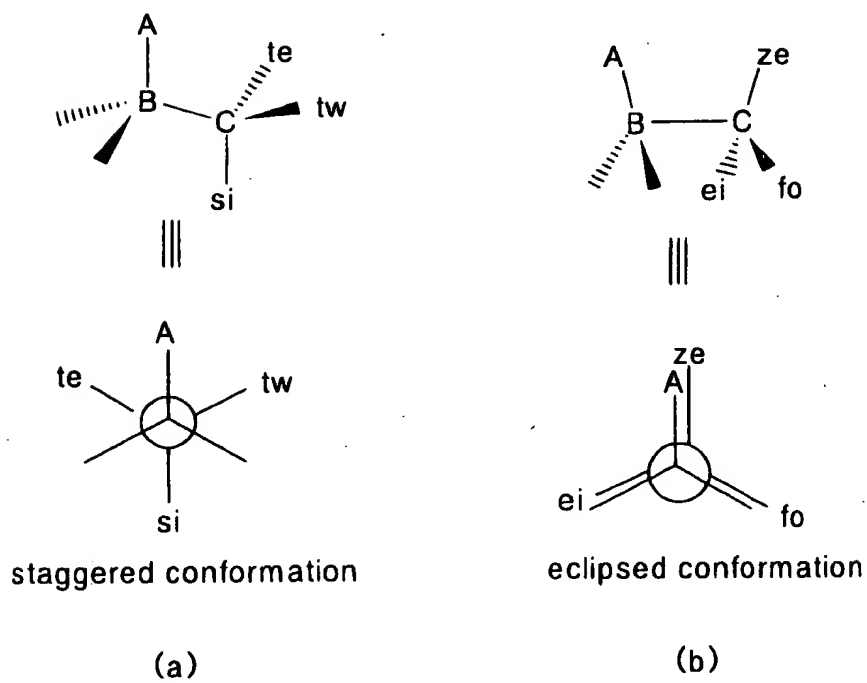
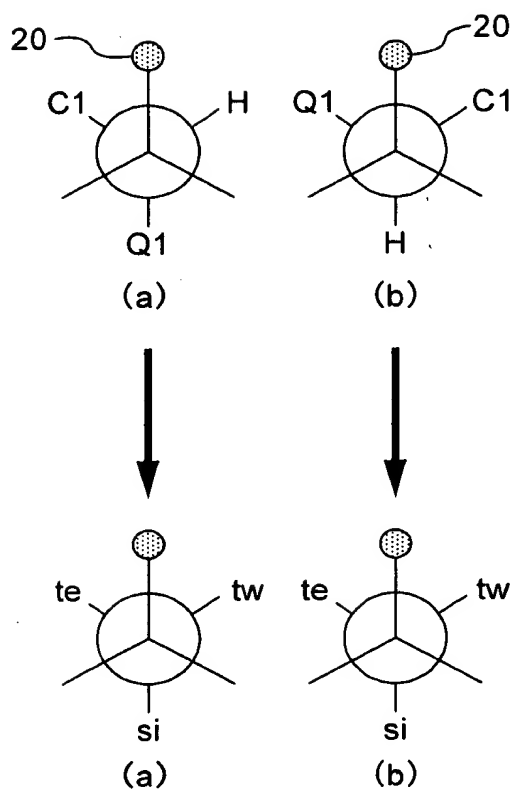


FIG. 7



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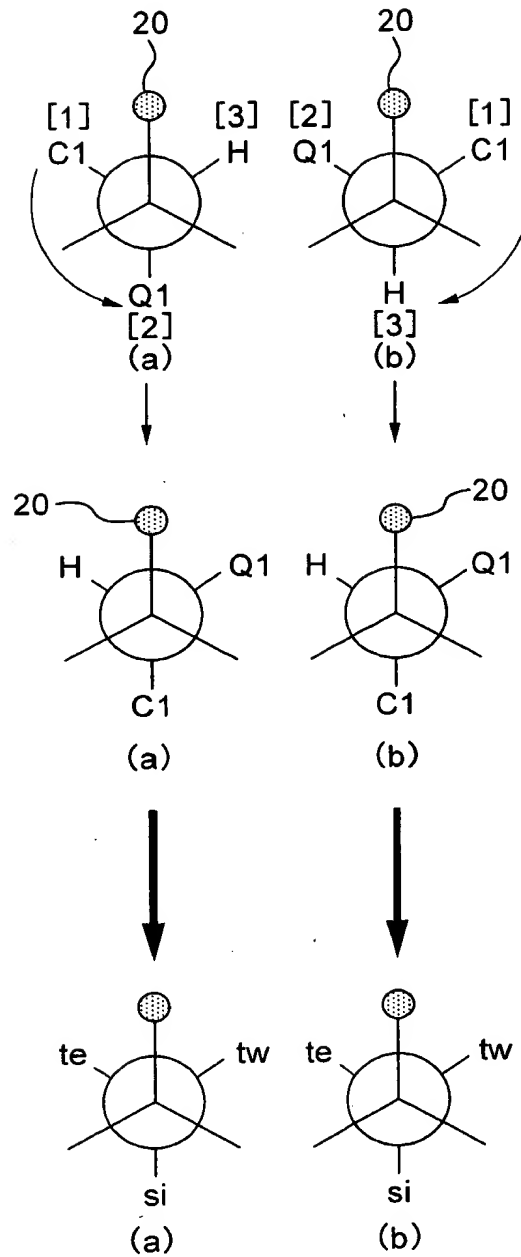
FIG. 8



CANOST Code	C1;Q1;H,
STEREO Code (a)	te;si;tw
STEREO Code (b)	tw;te;si

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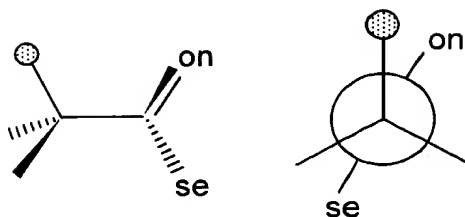
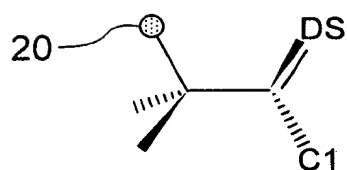
FIG. 9



CANOST Code	C1;Q1;H,
Configuration Identification Code (a)	si;tw;te
Configuration Identification Code (b)	si;tw;te

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FIG. 10

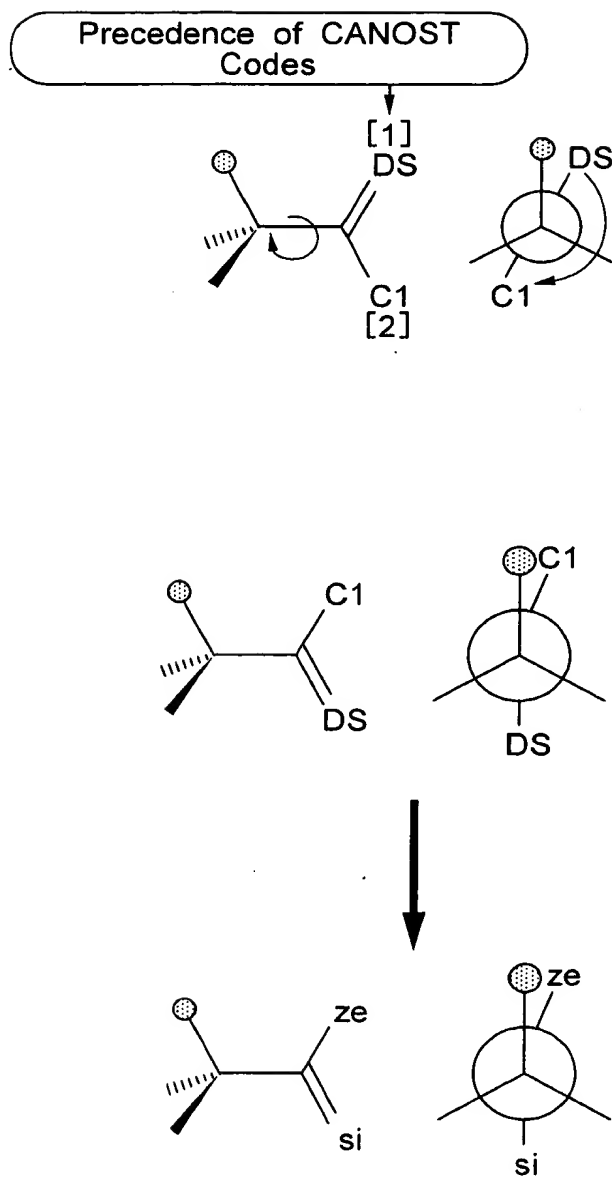


CANOST Code	DS;C1
STEREO Code	on;se

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FIG. 11



CANOST Code	DS;C1
Configuration Identification Code	si;ze

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FIG. 1 2

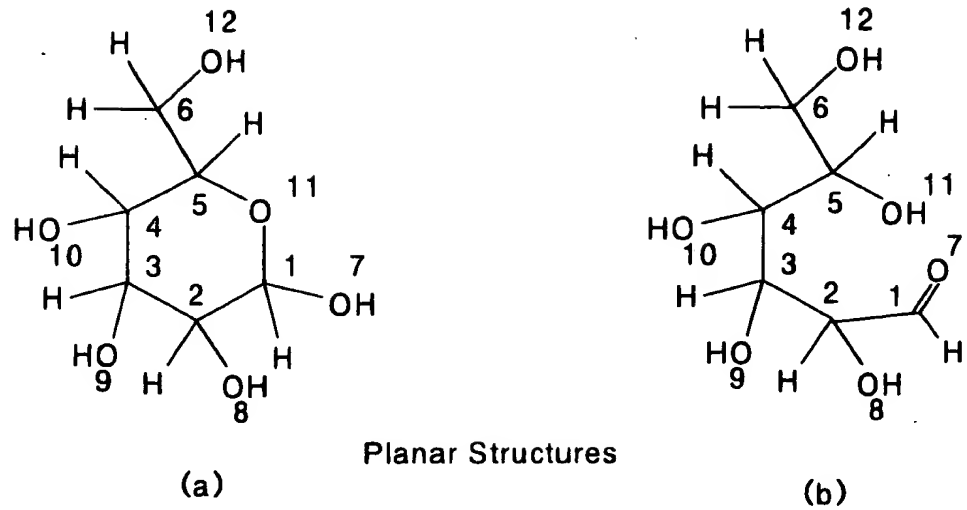


FIG. 1 3

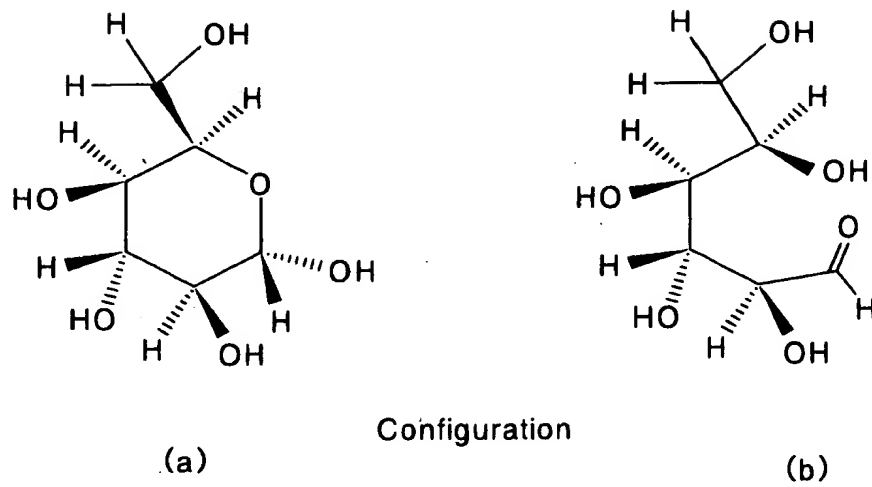
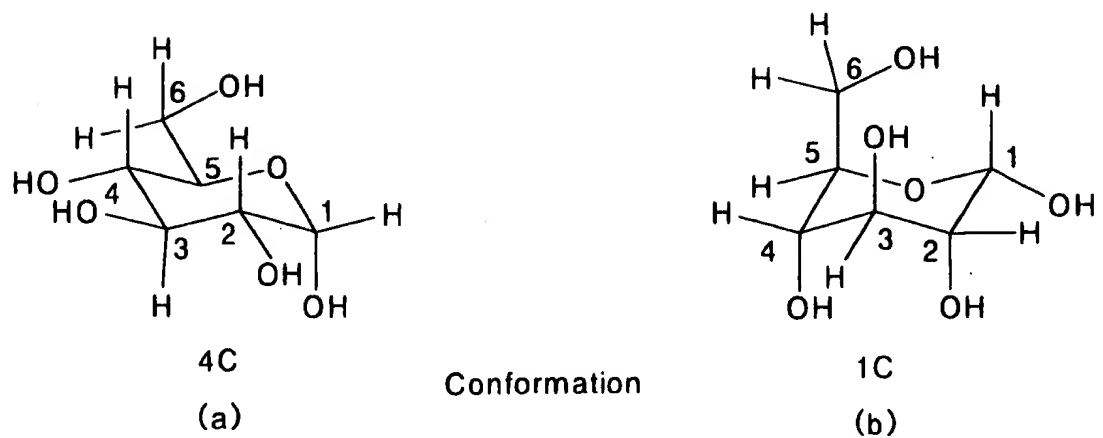


FIG. 1 4

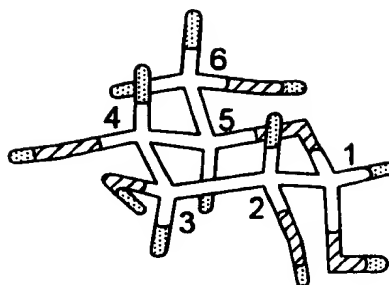


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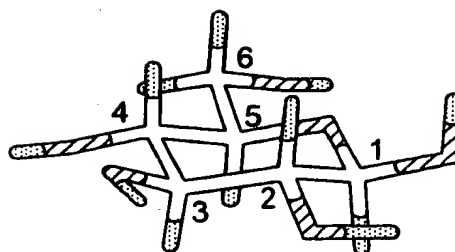
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FIG. 15

(a)

 α -glc 4C

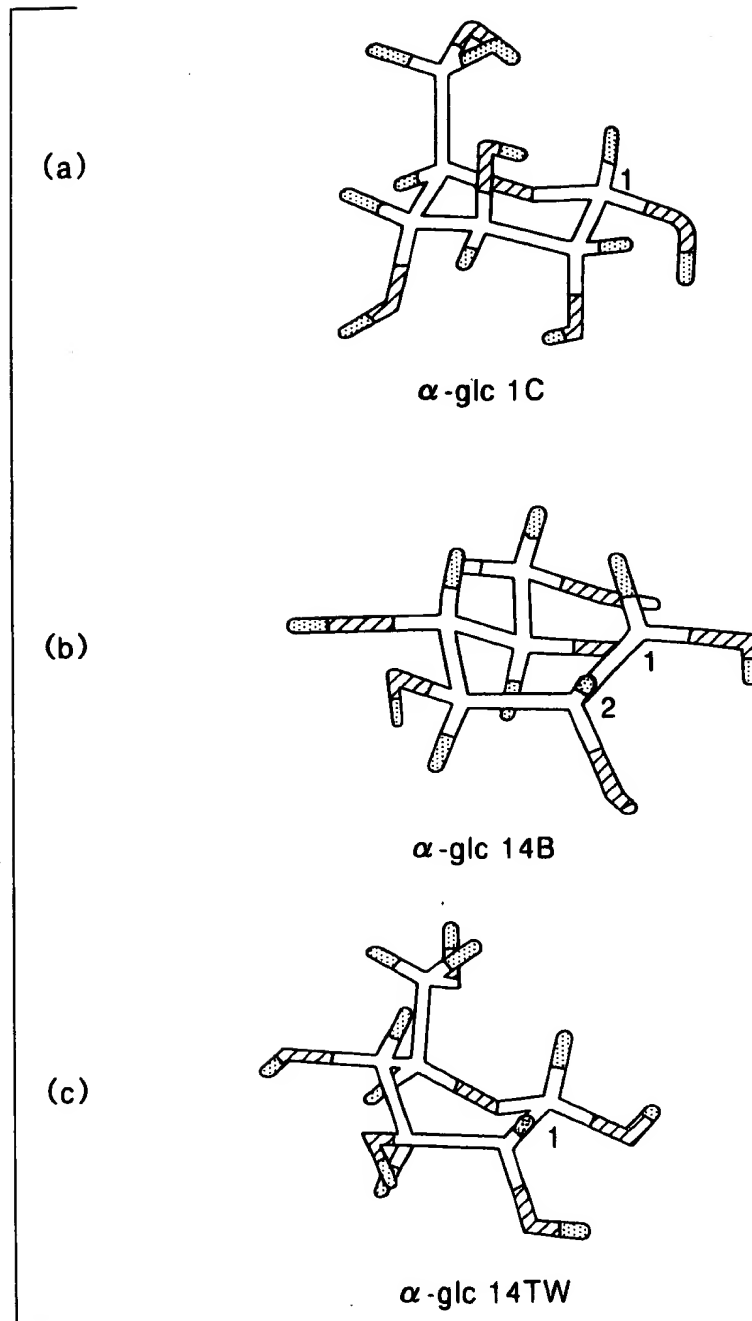
(b)

 β -glc 4C

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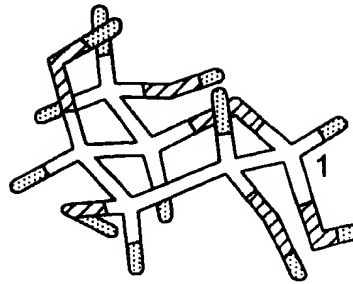
FIG. 16



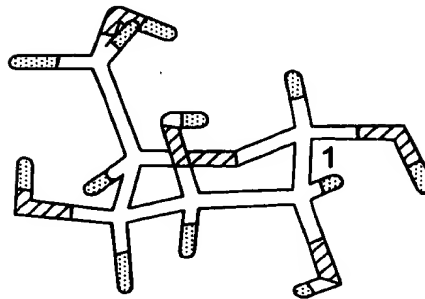
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FIG. 17

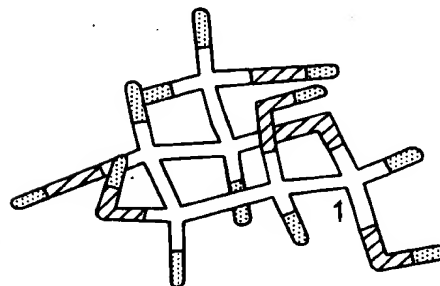
(a)

 α -gal 4C

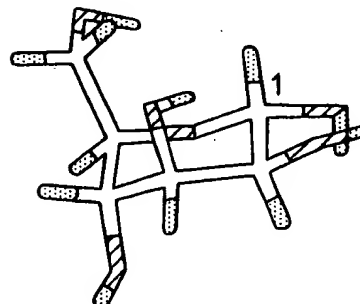
(b)

 α -gal 1C

(c)

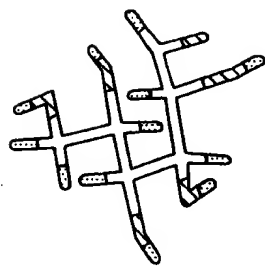
 α -man 4C

(d)

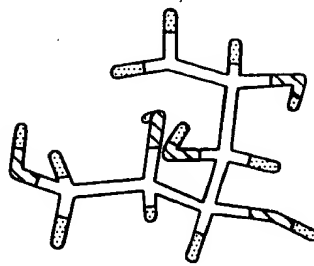
 α -man 1C

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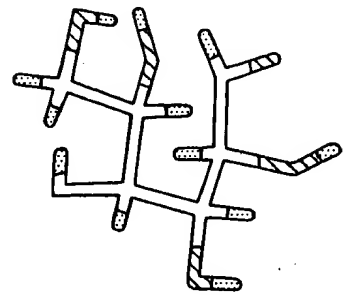
FIG. 18



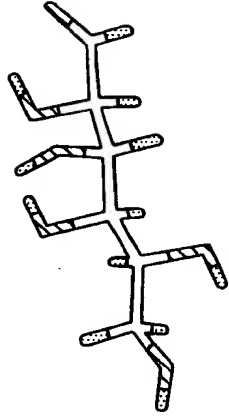
(a) α -glc 4C chain



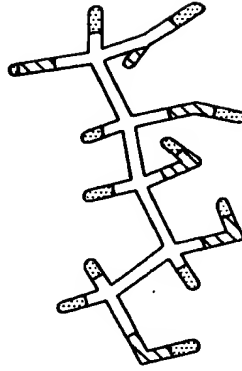
(b) α -glc 1C chain



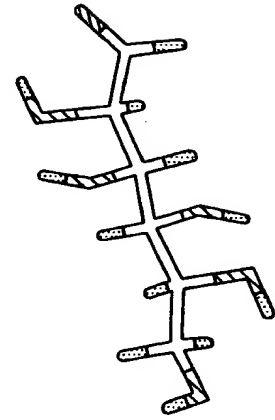
(c) α -gal 4C chain



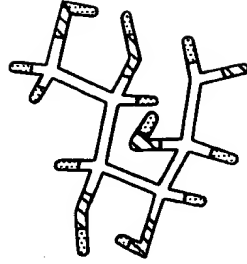
(d) α -glc 4C chain_linear



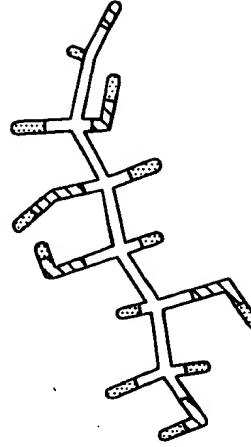
(e) α -glc 1C chain_H-bond



(f) α -gal 4C chain_linear



(g) α -man 4C chain



(h) α -man 4C chain_linear

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FIG. 19

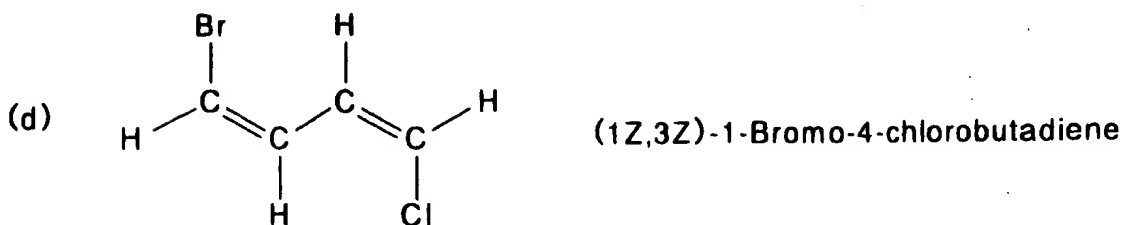
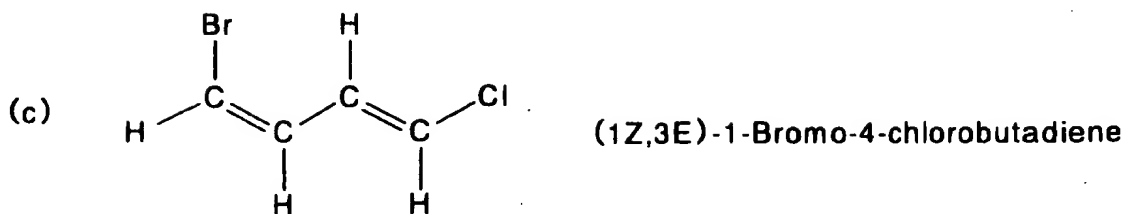
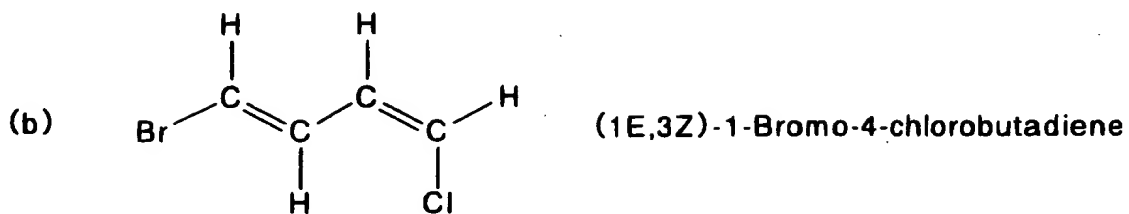
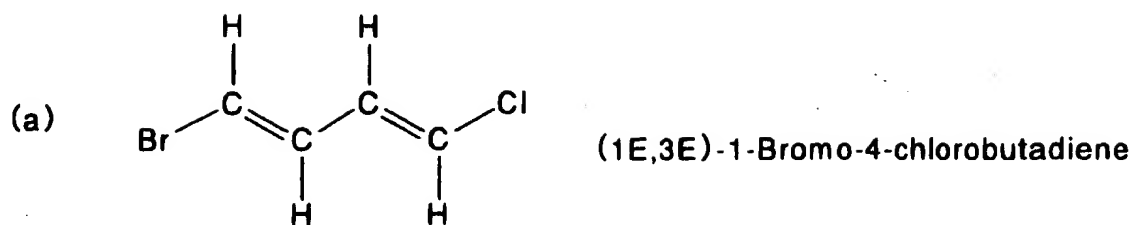


FIG. 20

a-Glc-4C

CANOST

- 1 C1*C1;Q:Q1:H*C1;Q1:H,C1,H,*C1;Q1:H,H,,&1;C2:H,*&1;Q1:H,H,,Q1:H,H,*H,,H,,*
- 2 C1*C1;C1;Q1:H*C1;Q1:H,Q:Q1:H,H,*C1;Q1:H,H,,&1,H,*&1;C2:H,H,,*,Q1:H,H,*H,,*
- 3 C1*C1;C1;Q1:H*C1;Q1:H,C1;Q1:H,H,*C2;Q:H,H,,&1;Q1:H,H,*Q1:H,H,&1,,,H,*H,,,*
- 4 C1*C1;C1;Q1:H*C1;Q1:H,C2;Q:H,H,*C1;Q1:H,H,,Q1:H,H,&1,,*&1;Q1:H,H,,H,,*,H,,*
- 5 C1*C1;C2;Q:H*C1;Q1:H,Q1:H,H,C1,*C1;Q1:H,H,H,,&1;Q1:H*&1;Q1:H,H,,,,H,*H,,,*
- 6 C2*C1;Q1:H:H*C1;Q:H,H,,*C1;Q1:H,C1,,*C1;Q1:H,H,,&1;Q1:H*&1;Q1:H,H,,,,H,*H,,,*
- 7 Q1*C1:H*C1;Q:H,*C1;Q1:H,C1,*C1;Q1:H,H,,&1;C2:H*&1;Q1:H,H,,Q1:H,H,*H,,H,,*
- 8 Q1*C1:H*C1;C1:H,*C1;Q1:H,Q:Q1:H,*C1;Q1:H,H,,&1,H,*&1;C2:H,H,,*,Q1:H,H,*H,,*
- 9 Q1*C1:H*C1;C1:H,*C1;Q1:H,C1;Q1:H,*C2;Q:H,H,,&1;Q1:H,H,*Q1:H,H,&1,,,H,*H,,,*
- 10 Q1*C1:H*C1;C1:H,*C1;Q1:H,C2;Q:H,*C1;Q1:H,H,,Q1:H,H,&1,*&1;Q1:H,H,,H,,*,H,,,*
- 11 Q*C1;C1*C1;C2:H,C1;Q1:H*C1;Q1:H,Q1:H,H,,&1;Q1:H,H,*&1;Q1:H,H,H,,H,,*,H,,,*
- 12 Q1*C2:H*C1;H;H,*C1;Q:H,,*C1;Q1;H,C1,*C1;Q1;H,H,,&1;Q1;H*&1;Q1;H,H,,,,H,*H,,*

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FIG. 20-1

Stereo

- 1 A*B;B;B*B*C;C;C,C,*te;si;tw,te,,tw;si;te,&l;si;te,te,,,tw;te;si,*tw,,te,*,
- 2 A*B;B;B*B*C;C;C,C,C,*tw;si;te,te,si,,&l;si;tw,tw,,,*,si;tw;te,,*te,,*,
- 3 A*B;B;B*B*C;C;C,C,C,*si;te;tw,tw,,tw;te;si,tw,*si;tw;te,&l,,,si,,,*,
- 4 A*B;B;B*B*C;C;C,C,C,*te;si;tw,si,,si;tw;te,tw,&l;te;si,tw,,te,,,*,si,,,*,
- 5 A*B;B;B*B*C;C;C,C,C,*tw;si;te,si,,te,te;tw;si*&l;si;tw,si,,,tw,*tw,,,*,
- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,,*,
- 7 A*B;B*C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;si;te,te,,,tw;te;si,*tw,,,te,*,
- 8 A*B;B*C;C;C,*si;tw;te,si;tw;te,*tw;si;te,te,,te,si,&l;si;tw,tw,,,*,si;tw;te,,*te,,*,
- 9 A*B;B*C;C;C,*si;te;tw,si;tw;te,*si;te;tw,tw,,tw;te;si,tw,*si;tw;te,&l,,,si,,,*,
- 10 A*B;B*C;C;C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;tw;te,tw,&l;te;si,tw,,te,,,*,si,,,*,
- 11 A*B;B*C;C;C,C,*te;si;tw,tw;te;si,,tw;si;te,tw,&l;si;te,si,,te,,,te,,,*,si,,,*,
- 12 A*B;B*C;C;C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,,*,

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FIG. 20-2

Configuration

- 1 A*B;B;B*B*C;C;C,C,*si;tw;te,si,,si;te;tw,*si;te;tw,si,,,si;tw;te,*si,,,si,*
- 2 A*B;B;B*B*C;C;C,C,*si;te;tw,si,,si,si,,*si;tw;te,si,,,*,si;tw;te,*si,,,*
- 3 A*B;B;B*B*C;C;C,C,*si;te;tw,si,,si;tw;te,si,,*si;tw;te,&l,,,si,,*si,,,*,
- 4 A*B;B;B*B*C;C;C,C,*si;tw;te,si,,si;tw;te,si,,*si;tw;te,si,,,*,si,,,*,
- 5 A*B;B;B*B*C;C;C,C,*si;te;tw,si,,si,,,si;te;tw*si;tw;te,si,,,*,si,*si,,,*
- 6 A*B;B;B*B*C;C;C,C,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,*,si,*si,,,*
- 7 A*B;B*B*C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,,*
- 8 A*B;B*B*C;C,*si;tw;te,si;tw;te,*si;te;tw,si,,si,si,*si;tw;te,si,,,*,si;tw;te,*si,,,*
- 9 A*B;B*B*C;C,*si;te;tw,si;tw;te,*si;te;tw,si,,si;tw;te,si,*si;tw;te,&l,,,si,,*si,,,*,
- 10 A*B;B*B*C;C,*si;te;tw,si;te;tw,*si;tw;te,si,,si;tw;te,si,*si;tw;te,si,,,*,si,,,*,
- 11 A*B;B*B*C;C,C,*si;tw;te,si;tw;te,,si;te;tw,si,*si;te;tw,si,,si,,,*,si,,,*,
- 12 A*B;B*B*C;C,*si;tw;te,,*si;tw;te,si,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,*,si,,,*,

FIG. 21

a-glc-4C

Stereo

- 1 A*B;B;B*B*C;C;C,C,*te;si;tw,te,,tw;si;te,&l;si;te,te,,,tw;te;si,*,tw,,,te,,*
- 2 A*B;B;B;B*B*C;C;C;C;C,C,*tw;si;te,te,,te,si,,&l;si;tw,tw,,,*,si;tw;te,*,te,,*
- 3 A*B;B;B;B*B*C;C;C;C;C,C,*si;te;tw,tw,,tw;te;si,tw,,*si;tw;te,&l,,,,si,,,*,te,,,*
- 4 A*B;B;B;B*B*C;C;C;C;C,C,*te;si;tw,si,,si;tw;te,tw,,&l;te;si,tw,,,te,,,*,si,,,*
- 5 A*B;B;B;B*B*C;C;C;C;C,C,*tw;si;te,si,,te,,,te;tw;si*&l;si;tw,si,,,,tw,*,tw,,,*
- 6 A*B;B;B;B*B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*,tw,,,*
- 7 A*B;B*B*C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;si;te,te,,,tw;te;si,*,tw,,,te,,*
- 8 A*B;B*B*C;C;C,*si;tw;te,si;tw;te,*tw;si;te,te,,te,si,&l;si;tw,tw,,,*,si;tw;te,*,te,,*
- 9 A*B;B*B*C;C;C,*si;te;tw,si;tw;te,*si;te;tw,tw,,tw;te;si,tw,*si;tw;te,&l,,,,si,,,*,te,,,*
- 10 A*B;B*B*C;C;C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;tw;te,tw,&l;te;si,tw,,,te,,,*,si,,,*
- 11 A*B;B*B*C;C;C;C;C,*te;si;tw,tw;te;si,,tw;si;te,tw,&l;si;te,si,,te,,,te,,,*,si,,,*
- 12 A*B;B*B*C;C;C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*,tw,,,*

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FIG. 21-1

a-gl c-4C

Stereo (CH₂→H)

- 1 A*B;B;B;B*C;C;C,C,*te;si;tw,te,,tw;si;te,&l;si;te,te,,,tw;H;H,*tw,,,te,,*
- 2 A*B;B;B;B*C;C;C,C,C,*tw;si;te,te,si,,&l;si;tw,tw,,,*,si;H;H,*te,,*
- 3 A*B;B;B;B*C;C;C,C,C,*si;te;tw,tw,tw;te;si,tw,,*si;H;H,&l,,,,si,,,te,,,,*
- 4 A*B;B;B;B*C;C;C,C,C,*te;si;tw,si,,si;H;H,tw,,&l;te;si,tw,,,te,,,*,si,,,*
- 5 A*B;B;B;B*C;C;C,C,C,*tw;si;te,si,,te,,,te;tw;si*&l;si;tw,si,,,,tw,*tw,,,*
- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,,tw,*tw,,,*
- 7 A*B;B*C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;si;te,te,,,tw;H;H,*tw,,,te,,*
- 8 A*B;B*C;C;C,*si;tw;te,si;tw;te,*tw;si;te,te,si,&l;si;tw,tw,,,*,si;H;H,*te,,*
- 9 A*B;B*C;C;C,*si;te;tw,si;tw;te,*si;te;tw,tw,,tw;te;si,tw,*si;H;H,&l,,,,si,,,te,,,,*
- 10 A*B;B*C;C;C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;H;H,tw,*&l;te;si,tw,,,te,,,*,si,,,*
- 11 A*B;B*C;C;C,C,*te;si;tw,tw;H;H,,tw;si;te,tw,*&l;si;te,si,,te,,,te,,,*,si,,,,*
- 12 A*B;B*C;C;C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,,*

FIG. 21-2

a-Glc-4C

Stereo(CH₂→H, OH→OH)

- 1 A*B;B;B;B*C;C;C,C,*te;si;tw,OH,,tw;si;te,&l;si;te,OH,,tw;H;H,*OH,,OH,,*
- 2 A*B;B;B;B*C;C;C,C,*tw;si;te,OH,,te,OH,,&l;si;tw,OH,,*,si;H;H,*OH,,*
- 3 A*B;B;B;B*C;C;C,C,*si;te;tw,OH,,tw;te;si,OH,,*si;H;H,&l,,*,OH,,*,OH,,*,*
- 4 A*B;B;B;B*C;C;C,C,*te;si;tw,OH,,si;H;H,tw,,&l;te;si,OH,,*,OH,,*,*
- 5 A*B;B;B;B*C;C;C,C,*tw;si;te,OH,,OH,,te;tw;si*&l;si;tw,OH,,*,OH,,*,*
- 6 A*B;B;B;B*C;C;C,C,*si;tw;te,si,,*tw;si;te,OH,,te;tw;si*&l;si;tw,OH,,*,OH,,*,*
- 7 A*B;B;B;B*C;C;C,*te;tw;si,OH,*te;si;tw,te,,tw;si;te*&l;si;te,OH,,*,tw;H;H,*OH,,*,*
- 8 A*B;B;B;B*C;C,C,*si;tw;te,si;tw;te,*tw;si;te,OH,,te,OH,&l;si;tw,OH,,*,si;H;H,*OH,,*
- 9 A*B;B;B;B*C;C,C,*si;te;tw,si;tw;te,*si;te;tw,OH,,tw;te;si,OH,*si;H;H,&l,,*,OH,,*,*
- 10 A*B;B;B;B*C;C,C,*si;te;tw,tw;si;te,*te;si;tw,OH,,si;H;H,tw,&l;te;si,OH,,*,OH,,*,*
- 11 A*B;B;B;B*C;C,C,C,*te;si;tw,tw;H;H,,tw;si;te,OH,&l;si;te,OH,,*,OH,,*,*
- 12 A*B;B;B;B*C;C,C,*si;tw;te,,*si;tw;te,si,*tw;si;te,OH,,te;tw;si*&l;si;tw,OH,,*,OH,,*,*

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FIG. 22

b-Glc-4C

Stereo

- 1 A*B;B;B*B*C;C;C,C,*te;si;tw,tw,,tw;si;te,&l;si;te,te,,,tw;si;te,*,tw,,,te,,*
- 2 A*B;B;B*B*C;C;C;C,C,*tw;si;te,te,,te,ni,&l;si;tw,tw,,,*,si;te;tw,*,te,,*
- 3 A*B;B;B*B*C;C;C;C,C,*si;te;tw,tw,,tw;si;te,si,*,si;te;tw,&l,,,ni,,,*,te,,,*
- 4 A*B;B;B*B*C;C;C;C,C,*te;si;tw,si,,si;te;tw,tw,,&l;si;te,si,,te,,,*,ni,,,,*
- 5 A*B;B;B*B*C;C;C;C,C,*tw;si;te,si,,te,,,te;si;tw&l;si;tw,si,,,,on,*,si,,,*
- 6 A*B;B;B*B*C;C;C,C,*si;tw;te,si,,*tw;si;te,si,,te;si;tw&l;si;tw,si,,,,on,*,si,,,*
- 7 A*B;B*B*C;C;C,*si;te;tw,si,*te;si;tw,tw,,tw;si;te&l;si;te,te,,,tw;si;te,*,tw,,,te,,*
- 8 A*B;B*B*C;C;C,*si;tw;te,si;te;tw,*tw;si;te,te,,te,ni,&l;si;tw,tw,,,*,si;te;tw,*,te,,*
- 9 A*B;B*B*C;C;C,*si;te;tw,si;tw;te,*si;te;tw,tw,,tw;si;te,si,*,si;te;tw,&l,,,ni,,,*,te,,,*
- 10 A*B;B*B*C;C;C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;te;tw,tw,&l;si;te,si,,te,,,*,ni,,,,*
- 11 A*B;B*B*C;C;C;C,*te;si;tw,tw;si;te,,tw;si;te,on,&l;si;te,si,,te,,,tw,,,*,si,,,*
- 12 A*B;B*B*C;C;C,*si;tw;te,,*,si;tw;te,si,*tw;si;te,si,,te;si;tw&l;si;tw,si,,,,on,*,si,,,,*

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FIG. 22-1

b-Glc-4C

Stereo (CH₂→H)

- 1 A*B;B;B;B*C;C;C,C,*te;si;tw,tw,tw;si;te,&l;si;te,te,,,tw;H;H,*tw,,,te,*,
- 2 A*B;B;B;B*C;C;C,C,C,*tw;si;te,te,te,ni,,&l;si;tw,tw,,,*,si;H;H,*te,*,
- 3 A*B;B;B;B*C;C;C,C,C,*si;te;tw,tw,tw;si;te,si,,*si;H;H,&l,,,ni,*te,,,*,
- 4 A*B;B;B;B*C;C;C,C,C,*te;si;tw,si,,si;H;H,tw,&l;si;te,si,,,te,,,*,ni,,,*,
- 5 A*B;B;B;B*C;C;C,C,C,*tw;si;te,si,,te,,,te;si;tw*&l;si;tw,si,,,,on,*si,,,*,
- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;si;tw*&l;si;tw,si,,,,on,*si,,,*,
- 7 A*B;B;B;B*C;C,C,*si;te;tw,si,*te;si;tw,tw,tw;si;te*&l;si;te,te,,,tw;H;H,*tw,,,te,,,*,
- 8 A*B;B;B;B*C;C,C,*si;tw;te,si;te;tw,*tw;si;te,te,te,ni,&l;si;tw,tw,,,*,si;H;H,*te,,,*,
- 9 A*B;B;B;B*C;C,C,*si;te;tw,si;tw;te,*si;te;tw,tw,tw;si;te,si,*si;H;H,&l,,,ni,*te,,,*,
- 10 A*B;B;B;B*C;C,C,*si;te;tw,tw;si;te,*te;si;tw,si,,si;H;H,tw,&l;si;te,si,,,te,,,*,ni,,,*,
- 11 A*B;B;B;B*C;C;C,C,*te;si;tw,tw;H;H,tw;si;te,ni,&l;si;te,si,,,te,,,*,si,,,*,
- 12 A*B;B;B;B*C;C,C,*si;tw;te,,*si;tw;te,si,*tw;si;te,si,,te;si;tw*&l;si;tw,si,,,,on,*si,,,*,

FIG. 22-2

b-Glc-4C

Stereo(CH₂→H, OH→OH)

- 1 A*B;B;B;B*C;C;C,C,*te;si;tw,OH,,tw;si;te,*&l;si;te,OH,,tw;H;H,*OH,,OH,,*
- 2 A*B;B;B;B*C;C;C,C,*tw;si;te,OH,,te,OH,*&l;si;tw,OH,,*,si;H;H,*OH,,*
- 3 A*B;B;B;B*C;C;C,C,*si;te;tw,OH,,tw;si;te,OH,,*si;H;H,&l,,OH,,*OH,,*,
- 4 A*B;B;B;B*C;C;C,C,*te;si;tw,OH,,si;H;H,tw,*&l;si;te,OH,,*,OH,,*,
- 5 A*B;B;B;B*C;C;C,C,*tw;si;te,OH,,te;si;tw*&l;si;tw,OH,,OH,*OH,,*,
- 6 A*B;B;B;B*C;C;C,C,*si;tw;te,si,,*tw;si;te,OH,,te;si;tw*&l;si;tw,OH,,OH,*OH,,*,
- 7 A*B;B;B;B*C;C,C,*si;te;tw,OH,*te;si;tw,tw,tw;si;te*&l;si;te,OH,,tw;H;H,*OH,,OH,,*
- 8 A*B;B;B;B*C;C,C,*si;tw;te,si;te;tw,*tw;si;te,OH,,te,OH,*&l;si;tw,OH,,*,si;H;H,*OH,,*
- 9 A*B;B;B;B*C;C,C,*si;te;tw,si;tw;te,*si;te;tw,OH,,tw;si;te,OH,*si;H;H,&l,,OH,*OH,,*,
- 10 A*B;B;B;B*C;C,C,*si;te;tw,tw;si;te,*te;si;tw,OH,,si;H;H,tw,*&l;si;te,OH,,OH,,*,OH,,*,
- 11 A*B;B;B;B*C;C,C,C,*te;si;tw,tw;H;H,,tw;si;te,OH,*&l;si;te,OH,,OH,,*,OH,,*,
- 12 A*B;B;B;B*C;C,C,*si;tw;te,,*si;tw;te,si,*tw;si;te,OH,,te;si;tw*&l;si;tw,OH,,OH,*OH,,*,

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FIG. 23

Comparison of a-Glc-4C with Stereo Code

a-Glc-4C

Stereo

6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,si,,te;tw;si*&l;si;tw,si,,,tw,*tw,,,*
 7 A*B;B;B;B*C;C;C,*te;tw;si,tw,*te;si;tw,te,,tw;si;te*&l;si;te,te,,,tw;te;si,*tw,,,te,,*

a-Glc-1C

Stereo

6 A*B;B;B;B*C;C;C,C,,*te;si;tw,tw,,*te;tw;si,si,,tw;si;te*&l;te;si,si,,,ni,*tw,,,*
 7 A*B;B;B;B*C;C;C,*si;te;tw,si,*tw;te;si,te,,te;tw;si*&l;tw;si,te,,,tw;te;si,*tw,,,te,,*

a-Glc-14B

Stereo

6 A*B;B;B;B*C;C;C,C,,*si;tw;te,fo,,*tw;si;te,si,,tw;si;te*&l;ei;fo,si,,,ni,*tw,,,*
 7 A*B;B;B;B*C;C;C,*si;te;tw,si,*ze;ei;fo,te,,ze;fo;ei*&l;si;te,te,,,tw;te;si,*tw,,,te,,*

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FIG. 23-1

a-Glc-14TB

Stereo

- 6 A*B;B;B;B;C;C;C;C,,*se:th:el,th,,*tw;si;te,si,,*tw:si:te*&l;se:th,si,,,tw,*fi,,*
7 A*B;B;C;C;C;C,*se:el:th,si,*el:se:th,on,el:th:se*&l;si;te,te,,,tw;te;si,*on,si,,*

b-Glc-4C

Stereo

- 6 A*B;B;B;B;C;C;C;C,,*si;tw;te,si,,*tw;si;te,si,,*te;si:tw*&l;si:tw,si,,,on,*si,,*
7 A*B;B;C;C;C;C,*si:te:tw,si,*te;si;tw,tw,tw;si;te*&l;si;te,te,,,tw;si:te,*tw,,te,,*

a-Gal-4C

Stereo

- 6 A*B;B;B;B;C;C;C;C,,*si;te:tw,si,,*tw;si;te,te,te;tw;si*&l;si:tw,si,,,tw,*tw,,*
7 A*B;B;C;C;C;C,*te:tw;si,tw,*te;si;tw,te,,tw;si;te*&l;te:si,te,,,tw;si:te,*tw,,te,,*

FIG. 23-2

a-Gal-1C

Stereo

6 A*B;B;B*B*C;C;C,,*te:tw:si,tw,,*te:tw:si,ni,,tw:si:te*&l:te:si,si,,,ni,*th,,,*
 7 A*B;B*B*C;C;C,*si:te:tw,si,*tw:te:si,te,,te:tw:si*&l;si;tw,te,,,tw:si:te,*on,,,el,,*

a-Man-4C

Stereo

6 A*B;B;B*B*C;C;C,,*si:tw:te,si,,*tw:si:te,si,,te:tw:si*&l:tw:si,ni,,,tw,*si,,,*
 7 A*B;B*B*C;C;C,*te:si:tw,tw,*te:si:tw,te,,tw:si:te*&l;si;te,on,,,tw:si:te,*tw,,,te,,*

a-Man-1C

Stereo

6 A*B;B;B*B*C;C;C,,*te:si:tw,tw,,*te:tw:si,si,,tw:si:te*&l:si;te,si,,,el,*si,,,*
 7 A*B;B*B*C;C;C,*si:tw:te,si,*tw:te:si,te,,te:tw:si*&l;tw:si,te,,,tw:si:te,*tw,,,te,,*

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Comparison of a-Glc-4C with Stereo Code (CH₂→H, OH→OH) FIG. 24

a-Glc-4C

StereoCH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*tw;si;te,OH,,te;tw;si*&l;si;tw,OH,,,,OH,*OH,,,*
7 A*B;B*C;C;C,*te;tw;si,OH,*te;si;tw,te,,tw;si;te*&l;si;te,OH,,,,tw;H;H,*OH,,OH,,,*

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a-Glc-1C

StereoCH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*te;si;tw,tw,,*te;tw;si,OH,,tw;si;te*&l;te;si,OH,,,,OH,*OH,,,*
7 A*B;B*C;C;C,*si;te;tw,OH,*tw;te;si,te,,te;tw;si*&l;tw;si,OH,,,,tw;H;H,*OH,,OH,,,*

a-Glc-14B

StereoCH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,fo,,*tw;si;te,OH,,tw;si;te*&l;ei;fo,OH,,,,OH,*OH,,,*
7 A*B;B*C;C;C,*si;te;tw,OH,*ze;ei;fo,te,,ze;fo;ei*&l;si;te,OH,,,,tw;H;H,*OH,,OH,,,*

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FIG. 24-1

a-Glc-14TB

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,,*se:th:el:th,,*tw:si;te,OH,,tw:si;te*&l;se:th,OH,,,OH,*OH,,,*

7 A*B;B;B;B*C;C,*se:el:th,OH,*el:se:th,on,,el:th;se*&l;si;te,OH,,,tw;H;H,*OH,,,OH,,*

b-Glc-4C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,,*si;tw;te,si,,*tw:si;te,OH,,te;si;tw*&l;si;tw,OH,,,OH,*OH,,,*

7 A*B;B;B;B*C;C,*si;te:tw,OH,*te;si;tw,tw,,tw;si;te*&l;si;te,OH,,,tw;H;H,*OH,,,OH,,*

a-Gal-4C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,,*si;te:tw,si,,*tw:si;te,OH,,te;tw;si*&l;si;tw,OH,,,OH,*OH,,,*

7 A*B;B;B;B*C;C,*te;tw;si,OH,*te;si;tw,te,,tw;si;te*&l;te;si,OH,,,tw;H;H,*OH,,,OH,,*

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FIG. 24-2

a-Gal-1C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,,*te:tw:si,tw,*te:tw:si,OH,,tw:si:te*&l:te:si,OH,,,OH,*,OH,,,*

7 A*B;B;B;C;C,*si:te:tw,OH,*tw:te:si,te,,te:tw:si*&l:si:tw,OH,,,tw:H;H,*,OH,,,OH,,,*

a-Man-4C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,*si:tw:te,si,*tw:si:te,OH,,te;tw:si*&l:tw:si,OH,,,OH,*,OH,,,*

7 A*B;B;B;C;C,*te:si:tw,OH,*te:si:tw,te,,tw;si:te*&l:si:te,OH,,,tw:H;H,*,OH,,,OH,,,*

a-Man-1C

StereoCH2→H, OH→OH)

6 A*B;B;B;B*C;C;C,*te:si:tw,tw,*te:tw:si,OH,,tw:si:te*&l:si:te,OH,,,OH,*,OH,,,*

7 A*B;B;B;C;C,*si:tw:te,OH,*tw:te:si,te,,te:tw:si*&l:tw:si,OH,,,tw:H;H,*,OH,,,OH,,,*

FIG. 25

Comparison of a-Glc-4C with Configuration Code

a-Glc-4C

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,*

a-Glc-1C

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,*

a-Glc-14B

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,*

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FIG. 25-1

a-Glc-14TB

Configuration

- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;tw;te,*si,,,si,,*

b-Glc-4C

Configuration

- 6 A*B;B;B;B*B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,si;tw;te*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;te;tw,si,,,si;te;tw,*si,,,si,,*

a-Gal-4C

Configuration

- 6 A*B;B;B;B*B*C;C;C,C,,*si;te;tw,si,,*si;te;tw,si,,si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,*si;te;tw,si,*si;tw;te,si,,si;te;tw*si;tw;te,si,,,si;te;tw,*si,,,si,,*

FIG. 25-2

a-Gal-1C

Configuration

- 6 A*B;B;B*B*C;C;C,C,,*si;te;tw,si,,*si;te;tw,si,,*si;te;tw*si;tw;te,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,C,,*si;te;tw,si,*si;tw;te,si,,*si;te;tw*si;tw;te,si,,,si;te;tw,*si,,,si,,*

a-Man-4C

Configuration

- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw*si;te;tw,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,C,,*si;tw;te,si,*si;tw;te,si,,*si;te;tw*si;te;tw,si,,,si;te;tw,*si,,,si,,*

a-Man-1C

Configuration

- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw*si;te;tw,si,,,si,*si,,,*
- 7 A*B;B*B*C;C;C,C,,*si;tw;te,si,*si;tw;te,si,,*si;te;tw*si;te;tw,si,,,si;te;tw,*si,,,si,,*

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FIG. 26

Comparison of a-Glc-4C-chain with Stereo Code

a-Glc-4C-chain

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,te,,*tw;si;te,si,,*te;si;tw,si,,*te;fi,th,,*
- 7 A*B*C;C*te;tw;si,*te;si;tw,el,*tw;si;te,te,,*si;te;tw,tw,,*si;tw;te,si,,*si,,,*

a-Glc-4C-chain-linear

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*si;tw;te,te,,*si;te;tw,si,,*si;tw;te,te,,*se;tw,fi,,*
- 7 A*B*C;C*se;ze;th,*si;tw;te,te,*,*si;te;tw,si,,*si;te;tw,tw,,*si;tw;te,si,,*si,,,*

a-Glc-1C-chain

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*te;si;tw,ni,,*te;tw;si,si,,*tw;te;si,si,,*si;tw,tw,,*
- 7 A*B*C;C*si;te;tw,*tw;te;si,te,*te;tw;si,te,,*te;tw;si,tw,,*si;tw;te,fo,,*te,,,*

FIG. 26-1

a-Glc-1C-chain-Hbond

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*te:si:tw,tw,,*si:te:tw,se,,*tw:te:si,el,,*ni:th,fo,,*
- 7 A*B*C;C*ni:on:fi,*tw:te:si,ze,*si:te:tw,th,,*te:tw:si,th,,*si:tw:te,te,*el,,,*

a-Gal-4C-chain

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*si:te:tw,el,,*tw:si:te,te,,*te:si:tw,si,,*te:fi,th,,*
- 7 A*B*C;C*te:tw:si,*te:si:tw,te,*tw:te:si,te,,*si:te:tw,tw,,*si:tw:te,si,,*tw,,,*

a-Gal-4C-chain-linear

Stereo

- 6 A*B;B;B*B*C;C;C,C,,*si:te:tw,te,,*si:te:tw,el,,*si:tw:te,ni,,*ei:tw,fi,,*
- 7 A*B*C;C*ei:ze:fo,*si:tw:te,on,*si:tw:te,on,,*si:te:tw,th,,*si:tw:te,si,,*tw,,,*

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FIG. 26-2

a-Man-4C-chain

Stereo

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,el,,*tw;si;te,si,,*te;tw;si,ni,,*te;fi,si,,*
- 7 A*B*C;C*te;si;tw,*te;si;tw,te,*tw;si;te,on,,*si;te;tw,tw,,*si;tw;te,se,,*tw,,,*

a-Man-4C-chain-linear

Stereo

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,el,,*si;te;tw,se,,*se;el;th,el,,*fo;te,ei,,*
- 7 A*B*C;C*fo;ze;ei,*se;th;el,ze,*si;te;tw,th,,*si;te;tw,th,,*si;tw;te,si,,*tw,,,*

CANOST

- 6 C2*C1;Q1;H;H*C1;Q1;H,H,,*C1;Q1;H,H,,*V1;Q1;H,H,,*QD;H,H,,*
- 7 QD*V1*C1;H*C1;Q1;H,*C1;Q1;H,H,*C1;Q1;H,H,,*Q1;H,H,H,,*H,,*

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FIG. 27

Comparison of a-Glc-4C-chain with Stereo Code (CH₂→H, OH→OH)

a-Glc-4C-chain

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,,*si;tw;te,OH,,*tw;si;te,OH,,*te;si;tw,OH,,*te;fi,OH,,*
- 7 A*B*C;C*te;tw;si,*te;si;tw,OH,*tw;si;te,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,*,

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a-Glc-4C-chain-linear

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,,*si;tw;te,OH,,*si;te;tw,OH,,*si;tw;te,OH,,*se;tw,OH,,*
- 7 A*B*C;C*se;ze;th,*si;tw;te,OH,*si;te;tw,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,*,

a-Glc-1C-chain

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,,*te;si;tw,OH,,*te;tw;si,OH,,*tw;te;si,OH,,*si;tw,OH,,*
- 7 A*B*C;C*si;te;tw,*tw;te;si,OH,*te;tw;si,OH,,*te;tw;si,OH,,*si;H;H,OH,,*OH,,*,

FIG. 27-1

a-Glc-1C-chain-Hbond

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*te:si:tw,OH,,*si:te:tw,OH,,*tw:te:si,OH,,*ni:th,OH,,*
- 7 A*B*C;C*ni:on:fi,*tw:te:si,OH,*si:te:tw,OH,,*te:tw:si,OH,,*si:H:H,OH,,*OH,,,*

a-Gal-4C-chain

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si:te:tw,OH,,*tw:si:te,OH,,*te:si:tw,OH,,*te:fi,OH,,*
- 7 A*B*C;C*te:tw:si,*te:si:tw,OH,*tw:te:si,OH,,*si:te:tw,OH,,*si:H:H,OH,,*OH,,,*

a-Gal-4C-chain-linear

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si:te:tw,OH,,*si:te:tw,OH,,*si:tw:te,OH,,*ei:tw,OH,,*
- 7 A*B*C;C*ei:ze:fo,*si:tw:te,OH,*si:tw:te,OH,,*si:te:tw,OH,,*si:H:H,OH,,*OH,,,*

FIG. 27-2

a-Man-4C-chain

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,OH,,*tw;si;te,OH,,*te;tw;si,OH,,*te;fi,OH,,*
- 7 A*B*C;C*te;si;tw,*te;si;tw,OH,*tw;si;te,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,,*

a-Man-4C-chain-linear

Stereo(CH₂→H, OH→OH)

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,OH,,*si;te;tw,OH,,*se;el;th,OH,,*fo;te,OH,,*
- 7 A*B*C;C*fo;ze;ei,*se;th;el,OH,*si;te;tw,OH,,*si;te;tw,OH,,*si;H;H,OH,,*OH,,,*

CANOST

- 6 C2*C1;Q1;H;H*C1;Q1;H,H,,*C1;Q1;H,H,,*V1;Q1;H,H,,*QD;H,H,,*
- 7 QD*V1*C1;H*C1;Q1;H,*C1;Q1;H,H,*C1;Q1;H,H,,*C2;Q1;H,H,,*Q1;H;H,H,,*H,,,*

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FIG. 28

Comparison of a-Glc-4C-chain with Configuration Code

a-Glc-4C-chain

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;te;tw,si,,*si;tw;te,si,,*si,,*

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a-Glc-4C-chain-linear

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;te;tw,si,,*si;tw;te,si,,*si,,*

a-Glc-1C-chain

Configuration

- 6 A*B;B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;te;tw,si,,*si;tw;te,si,,*si,,*

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FIG. 28-1

a-Glc-1C-chain-Hbond

Configuration

- 6 A*B:B;B;B*C;C;C,C,,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,,*

a-Gal-4C-chain

Configuration

- 6 A*B:B;B;B*C;C;C,C,,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,,*

a-Gal-4C-chain-linear

Configuration

- 6 A*B:B;B;B*C;C;C,C,,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si;ze,si,,*
- 7 A*B*C;C*si;te;tw,*si;tw;te,si,*si;tw;te,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,,*

FIG. 28-2

a-Man-4C-chain

Configuration

- 6 A*B;B;B;B*C;C;C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw,si,,*si;ze,si,,*
- 7 A*B*C;C*si;tw;te,*si;tw;te,si,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,*

a-Man-4C-chain-linear

Configuration

- 6 A*B;B;B;B*C;C;C,,*si;tw;te,si,,*si;te;tw,si,,*si;te;tw,si,,*si;ze,si,,*
- 7 A*B*C;C*si;tw;te,*si;tw;te,si,*si;te;tw,si,,*si;te;tw,si,,*si;tw;te,si,,*si,,*

CANOST

- 6 C2*C1;Q1;H;H*C1;Q1;H,H,,*C1;Q1;H,H,,*V1;Q1;H,H,,*QD;H,H,,*
- 7 QD*V1*C1;H*C1;Q1;H,*C1;Q1;H,H,*C1;Q1;H,H,,*C2;Q1;H,H,,*Q1;H;H,H,,*H,,*

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FIG. 29

Comparison of 1Br4Cl_butadiene isoers

CANOST

Br LB*D1*D1;H*D1;H,*D1;H,*LC;H,*

Cl LC*D1*D1;H*D1;H,*D1;H,*LB;H,*

1E3E1Br4Cl_butadiene

Stereo

Br A*B*C;C*si;ze,*si;ze,*si;ze,*

Cl A*B*C;C*si;ze,*si;ze,*si;ze,*

Configuration

Br A*B*C;C*si;ze,*si;ze,*si;ze,*

Cl A*B*C;C*si;ze,*si;ze,*si;ze,*

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1E3Z1Br4Cl_butadiene FIG. 29-1

Stereo

Br A*B*C;C*si;ze,*si;ze,*ze;si,*Cl A*B*C;C*ze;si,*si;ze,*si;ze, *

Configuration

Br A*B*C;C*si;ze,*si;ze,*ze;si,*Cl A*B*C;C*ze;si,*si;ze,*si;ze, *

1Z3E1Br4Cl_butadiene

Stereo

Br A*B*C;C*ze;si,*si;ze,*si;ze, *Cl A*B*C;C*si;ze,*si;ze,*ze;si,*

Configuration

Br A*B*C;C*ze;si,*si;ze,*si;ze, *Cl A*B*C;C*si;ze,*si;ze,*ze;si,*

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FIG. 29-2

1Z3Z1Br4Cl_butadiene

Stereo

Br A*B*C;C*ze;si,*si;ze,*ze;si,*Cl A*B*C;C*ze;si,*si;ze,*ze;si,*

Configuration

Br A*B*C;C*ze;si,*si;ze,*ze;si,*Cl A*B*C;C*ze;si,*si;ze,*ze;si,*

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FIG. 30

